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2012 EPL 98 50004

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Active Brownian particles in two-dimensional traps

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received 4 April 2012; accepted in final form 14 May 2012

published online 12 June 2012

PACS 05.40.-a – Statistical physics, thermodynamics, and nonlinear dynamical systems:
Fluctuation phenomena, random processes, noise, and Brownian motion

PACS 87.10.Mn – Biological and medical physics: Stochastic modeling

PACS 87.17.Jj – Cell locomotion, chemotaxis

Abstract – We consider a population of self-propelled Brownian particles in 2D traps. For non-interacting particles the stationary distribution for position and orientation is found analytically for small and large rotational diffusivities. These results are used to map the system of interacting active particles onto a system of passive particles in a modified trapping potential which we then formulate as a dynamic density functional theory. Our approach is supported by Brownian dynamics simulations of the original and the effective model.

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Introduction. – Individual and collective properties of self-propelled particles, such as swimming bacteria, moving in confined geometries or traps, have recently attracted much interest from both the experimental [1–3] and modeling [4–12] point of view.

Despite some recent progress in the theory of a single active particle [5,6,11,13], the analytical description of the non-equilibrium dynamics of many interacting active particles is an open and challenging problem. Particle interactions are typically treated numerically by directly solving the system of equations for individual particles (see, for example, [7,8,14]). From a phenomenological point of view, interactions between particles can be described in the framework of the so-called drift-diffusion model [10] by assuming that various physical parameters such as the propulsion velocity and the tumbling rate are known functions of the local particle density. A similar phenomenological approach in combination with lattice models has been used to study the effect of far-field hydrodynamic interactions [12,15,16].

A much more powerful and universal way of describing the dynamics of many interacting particles boils down to deriving the Smoluchowski or Boltzmann equation for the one-body probability density. Several recent works attacked the problem along this path. For example, in ref. [17] the Boltzmann equation for self-propelled point

particles moving in 2D was obtained under the assumption of binary collisions. A system of many self-propelled hard rods was studied in refs. [9,18], where the particle interaction was treated using the mean-field Onsager functional. Typically, the mean-field approximation assumes that the two-body density can be written as the product of two one-body densities. It underestimates particle correlations and thereby is limited to low packing fractions where correlations are weak.

A more systematic way of dealing with particle interactions is to resort to dynamic density functional theory (DDFT) [19–21]. The key ingredient of DDFT is the equilibrium excess free energy functional $F_{\text{ex}}[\rho(\mathbf{r}, t)]$ which describes the interaction energy of particles in equilibrium. Deriving $F_{\text{ex}}[\rho(\mathbf{r}, t)]$ in terms of the one-body distribution $\rho(\mathbf{r}, t)$ is a non-trivial problem of statistical physics. It requires elaborate computations which essentially boil down to computing the partition function in the canonical or grand canonical ensemble [22,23]. Alternatively, one applies general considerations based on measure theory to derive the excess free energy for hard spheres or rods [24–27].

Our knowledge of the equilibrium $F_{\text{ex}}[\rho(\mathbf{r}, t)]$ is very scarce and is only available for very few systems of passive colloidal particles. Furthermore, DDFT for passive colloids assumes that local particle correlations can be described by the equilibrium $F_{\text{ex}}[\rho(\mathbf{r}, t)]$ [19–21]. If one applies this assumption also to active particles, then a straightforward

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generalization of DDFT to active particles arises [18]. An alternative approach was outlined quite recently in ref. [13]. When a non-equilibrium steady state exists, one can formally assign to it an effective free energy in the one-body density and formulate a DDFT for active particles based on such an effective free energy. For a single particle this approach is straightforward, for interacting active particles it is even more complex than determining the equilibrium $F_{\text{ex}}[\rho(\mathbf{r}, t)]$.

In view of the above, we derive here an easy tractable Smoluchowski equation for the one-body density, which describes the dynamics of the spatial distribution of active particles in 2D traps interacting via a steric pair potential. In doing so, we map the original system of active particles onto an effective system of passive particles moving in a modified trapping potential. In the resulting Smoluchowski equation the correlations between particles are taken into account via the excess free energy of passive particles, whereas the active component of the dynamics enters the equation in the form of an effective external potential. In order to compute the latter, we derive an analytic expression for the stationary density of non-interacting particles in cases of small and large rotational diffusion coefficients and use it to compute the average orientation of the active particles. The analytical results are tested on the example of active hard discs. We approximate their interactions by a steric or soft-core potential. We start with setting up the problem and solve the single-particle system first.

Overdamped motion of active colloids. – Following ref. [13], we consider the overdamped motion of a single active Brownian particle with the coordinate \mathbf{r} , propulsion velocity v_0 , and the direction of active motion given by the unit vector \mathbf{p} . In a trapping potential $U(\mathbf{r})$, the overdamped motion is described by a set of two Langevin equations,

$$\dot{\mathbf{r}} = -\mu\nabla U + v_0\mathbf{p} + \boldsymbol{\xi}(t), \quad \dot{\mathbf{p}} = \boldsymbol{\eta}(t) \times \mathbf{p}, \quad (1)$$

where the stochastic terms $\boldsymbol{\xi}(t)$ and $\boldsymbol{\eta}(t)$ represent translational and rotational noise, respectively. They fulfill the fluctuation-dissipation relations $\langle \boldsymbol{\xi}(t)\boldsymbol{\xi}(t') \rangle = 2\mu k_B T \delta(t-t')$ and $\langle \boldsymbol{\eta}(t)\boldsymbol{\eta}(t') \rangle = 2D_r \delta(t-t')$ with translational mobility μ and rotational diffusivity D_r . Note that unlike in ref. [13], the coefficient D_r is not necessarily of thermal origin. Rather, we consider it here as an independent parameter, which might or might not be temperature dependent. For instance, in case of a bacterium performing a run-and-tumble motion, D_r is linked to the tumbling rate. As a result, the bacterium exhibits diffusive motion on time scales larger than the typical time between two subsequent tumbles [10].

When treated in the Stratonovich interpretation, eqs. (1) yield the Smoluchowski equation for the probability density $\rho(\mathbf{r}, \mathbf{p}, t)$,

$$\partial_t \rho + \nabla \cdot \mathbf{J}_t + \mathbf{R} \cdot \mathbf{J}_{\text{rot}} = 0, \quad (2)$$

with the rotation operator $\mathbf{R} = \mathbf{p} \times \nabla_{\mathbf{p}}$ and the translational and rotational probability currents given by $\mathbf{J}_t = [v_0\mathbf{p} - \mu\nabla U(\mathbf{r})]\rho - \mu k_B T \nabla \rho$ and $\mathbf{J}_{\text{rot}} = -D_r \mathbf{R}\rho$, respectively. Equation (2) is clear since it is the continuity equation for the probability and the currents contain typical diffusion and drift terms. The Smoluchowski equation (2) was also derived in ref. [13] as the overdamped limit of the Langevin equations for a single active particle with inertia in a viscous fluid.

It is instructive to compare eqs.(1) with the one-dimensional diffusion-drift model of the run-and-tumble particles of ref. [10]. On the one hand, eqs.(1) or (2) predict a total diffusivity D_{tot} of an active colloidal particle given by $D_{\text{tot}} = \mu k_B T + v_0^2 D_r^{-1}$. On the other hand, as it was shown in ref. [10], the total diffusivity of a run-and-tumble particle measured on times much larger than the inverse tumbling rate D_r^{-1} is proportional to the square of the drift velocity v_0 , *i.e.*, $D_{\text{tot}} = v_0^2 D_r^{-1}$. As a consequence, both models coincide for $T=0$ and the diffusion-drift model is incomplete when the thermal diffusivity $\mu k_B T$ becomes comparable to $v_0^2 D_r^{-1}$.

Further on, we rescale \mathbf{r} with the diameter of the particle d and t with the characteristic thermal diffusion time $d^2(\mu k_B T)^{-1}$. The rescaled probability currents from eq. (2) (denoted by tildas) read

$$\tilde{\mathbf{J}}_t = \left[\text{Pe} \mathbf{p} - \tilde{\nabla} \tilde{U}(\tilde{\mathbf{r}}) \right] \rho - \tilde{\nabla} \rho, \quad \tilde{\mathbf{J}}_{\text{rot}} = -\tilde{D}_r \tilde{\mathbf{R}} \rho, \quad (3)$$

with the rescaled potential $\tilde{U} = (1/k_B T)U(d\tilde{\mathbf{r}})$, rotational diffusivity $\tilde{D}_r = (d^2 D_r)/(\mu k_B T)$, and the Peclet number $\text{Pe} = (dv_0)/(\mu k_B T)$, which compares active to diffusive motion. For the sake of simplicity we omit “tildas” in all equations below.

Single particle in 2D traps with radial symmetry.

– In case of a two-dimensional trap which we mimic by the trapping potential $U(\mathbf{r})$, the unit vector $\mathbf{p} = (\cos \alpha, \sin \alpha)$ can be replaced by the local angle α between \mathbf{p} in point \mathbf{r} and the x -axis. The rotational operator simplifies to $\mathbf{R} \cdot \mathbf{R} = \partial^2/\partial \alpha^2$, which corresponds to the standard diffusion of the angle α on the unit circle with diffusivity D_r .

If $U(\mathbf{r})$ is radially symmetric, the dimensionless Smoluchowski equation (2) can be conveniently written in polar coordinates (r, ϕ) ,

$$\partial_t \rho + \frac{1}{r} \frac{\partial (r J_r)}{\partial r} + \frac{1}{r} \frac{\partial J_\phi}{\partial \phi} - D_r \frac{\partial^2 \rho}{\partial \alpha^2} = 0. \quad (4)$$

The radial and angular components of the translational probability fluxes are given by $J_r = -\partial_r \rho - (\partial_r U)\rho + \text{Pe} \cos(\phi - \alpha)\rho$ and $J_\phi = -(1/r)\partial_\phi \rho + \text{Pe} \sin(\phi - \alpha)\rho$, respectively. Because of the radial symmetry, the stationary solution ($\partial_t \rho = 0$) of eq. (4) $\rho_s(r, \phi, \alpha)$ can only depend on the difference $\phi - \alpha$ and not on ϕ and α separately. In fact the integrated distribution $\int_0^{2\pi} \rho_s(r, \phi, \alpha) d\alpha = f(r)$ should not depend on the polar angle ϕ . This condition is automatically satisfied if ρ_s is a 2π periodic function of $\phi - \alpha$.

Introducing the effective potential $U^{\text{eff}} = U(r) - \text{Pe} \cos(\psi)$ with $\psi = \alpha - \phi$, the stationary density $\rho_s(r, \psi)$ satisfies the continuity equation

$$\text{div} \mathbf{J}_s^{\text{eff}} = 0, \quad (5)$$

The operator “div” is taken in polar coordinates (r, ψ) and the effective stationary radial and angular probability fluxes are

$$\begin{aligned} (\mathbf{J}_s^{\text{eff}})_r &= -\partial_r \rho_s - (\partial_r U^{\text{eff}}) \rho_s, \\ r(\mathbf{J}_s^{\text{eff}})_\psi &= -[D_r r^2 + 1] \partial_\psi \rho_s - (\partial_\psi U^{\text{eff}}) \rho_s. \end{aligned} \quad (6)$$

Remarkably, neither the probability fluxes of eqs. (3), nor the effective fluxes of eqs. (6) necessarily vanish in the stationary state. Equation (5) merely implies that $(\mathbf{J}_s^{\text{eff}})_r = (1/r) \partial_\psi A$ and $(\mathbf{J}_s^{\text{eff}})_\psi = -\partial_r A$, where $A(r, \psi)$ is an arbitrary scalar field. As a consequence, eqs. (6) cannot be integrated generally to yield a closed form of ρ_s . However, an asymptotic expression for ρ_s can be obtained for an arbitrary radially symmetric potential $U(r)$ in case of a small and large rotational diffusivity D_r .

Limit of small rotational diffusivity. First consider the case, when the rotational diffusion time D_r^{-1} is large compared to the time needed by a particle to move radially to its equilibrium position r_0 which is determined by the condition $\text{Pe} = \partial_r U(r_0)$. Without noise the particle approaches r_0 exponentially, $r(t) - r_0 \sim \exp(-t \partial_r^2 U(r_0))$, with the characteristic run-up time $\tau_r = [\partial_r^2 U(r_0)]^{-1}$.

As $D_r^{-1} \gg \tau_r$, the rotational flux in eqs. (3) disappears and the translational flux in eqs. (3) determines the effective fluxes in eqs. (6). This implies that the active particle behaves as a passive spherical particle, which moves in the effective potential U^{eff} . The zeroth-order solution $\rho_s^{(0)} \sim O(D_r^0)$ of $\mathbf{J}_s^{\text{eff}} = 0$ with the flux components of eqs. (6) then becomes

$$\rho_s^{(0)} = C e^{-U(r) + \text{Pe} r \cos \psi}, \quad (7)$$

where $C = [\int_0^{2\pi} d\psi \int_0^\infty dr (r e^{-U(r) + \text{Pe} r \cos \psi})]^{-1}$ is the normalization constant. Notice that $\rho_s^{(0)}$ remains bounded only if $\lim_{r \rightarrow \infty} U(r) - \text{Pe} r = \infty$. For fixed r , $\rho_s^{(0)}$ is maximal for $\psi = \phi - \alpha = 0$ which implies that the particles move, on average, away from the center of the trap and thereby exhibit polar order.

The radial distribution $\tilde{\rho}_s^{(0)}(r) = \int_0^{2\pi} \rho_s^{(0)} d\psi$ is obtained as

$$\tilde{\rho}_s^{(0)}(r) = 2\pi C e^{-U(r)} I_0(\text{Pe} r), \quad (8)$$

where $I_0(x)$ is the modified Bessel function of the first kind.

At small Péclet number, the radial distribution $\tilde{\rho}_s^{(0)}(r)$ is bell-shaped with a maximum in the center at $r = 0$. So, the particles spend most of the time around the center of the trap and we call this case the strong trapping regime. Increasing Pe , a transition to the weak trapping regime occurs where $\tilde{\rho}_s^{(0)}(r)$ develops a local minimum in the center and a maximum at a nonzero radius ($r_m \neq 0$).

The transition is located at a critical Péclet number $\text{Pe}^{(c)} = \sqrt{2U''(0)}$. Note that for non-harmonic potentials, weak trapping is visible for arbitrarily small activity of the active particles when $U''(0) = 0$. Our results qualitatively agree with the findings of the diffusion-drift model [10]¹.

Limit of large rotational diffusivity. At any constant Pe no matter how large, the distribution of particles concentrated on a ring with nonzero radius transforms into a bell-shaped $\tilde{\rho}_s(r)$ centered at $r = 0$ as the rotational diffusivity D_r exceeds a critical value $D_r^{(c)}(\text{Pe})$.

In order to study this case systematically, we set

$$\rho_s(r, \psi) = e^{-U(r)} \left(f^{(0)} + f^{(1)} + f^{(2)} + \dots \right), \quad (9)$$

where $f^{(i)}$ is of the order of $(1/D_r)^i$. Substituting this series in eq. (5) and using standard methods of asymptotic expansions, we obtain up to the first order in $1/D_r$

$$f^{(0)} = c, \quad f^{(1)} = c \text{Pe} \partial_r U(r) \cos \psi + a(r), \quad (10)$$

where c and $a(r)$ are some unknown constant and function, respectively.

In order to determine $a(r)$, we recall that $(\mathbf{J}_s^{\text{eff}})_r = (1/r) \partial_\psi A(r, \psi)$ with some $A(r, \psi)$ periodic in ψ implying that the integral $\int_0^{2\pi} (\mathbf{J}_s^{\text{eff}})_r d\psi$ vanishes in any order of $1/D_r$. This yields $a(r) = c(\text{Pe}^2/2)U(r)$ and the stationary density becomes

$$\rho_s = c e^{-U(r)} \left(1 + \frac{2\text{Pe} \partial_r U(r) \cos \psi + \text{Pe}^2 U(r)}{2D_r} + O(D_r^{-2}) \right). \quad (11)$$

By integrating over ψ , we obtain the radial density

$$\tilde{\rho}_s = 2\pi c e^{-U(r)} \left(1 + \frac{\text{Pe}^2 U(r)}{2D_r} + O(D_r^{-2}) \right), \quad (12)$$

with the constant c determined from the normalization condition $\int_0^\infty r \tilde{\rho}_s(r) dr = 1$.

The asymptotic expansion of eq. (12) is valid if the second term on the right-hand side computed at a characteristic radius with $U(r_c) = 1$ is significantly smaller than the first term, *i.e.*, when $\text{Pe}^2/D_r \ll 1$. From eq. (12) we determine the critical rotational diffusivity $D_r^{(c)} = \text{Pe}^2/2$, where the transition from strong to weak trapping occurs. Unfortunately, this value of $D_r^{(c)}$ also implies that the expansion of in eq. (12) is no longer valid.

As an example we consider a radially symmetric harmonic trap with a potential $U(r) = \gamma r^2$ in reduced units. The solid lines in fig. 1(a) show the stationary radial distribution $\tilde{\rho}_s(r)$ for different Péclet numbers Pe as obtained from numerical simulation of the dimensionless Langevin equations (1) using the parameters $\gamma = 10$ and $D_r = 1$. The dashed lines represent the analytical density of eq. (8). Since for this choice of parameters the characteristic rotational diffusion time $(D_r)^{-1} = 1$

¹Note that our definition of weak/strong trapping is opposite to the definition used in ref. [10] within the drift-diffusion model.

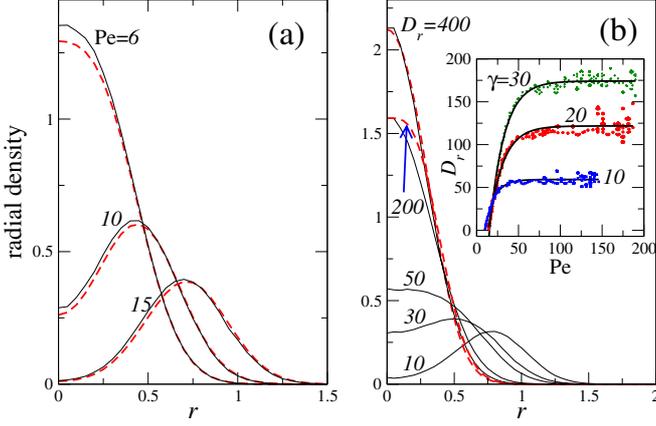


Fig. 1: (Color online) (a) Transition from strong to weak trapping for increasing Péclet number Pe demonstrated in the limit of small rotational diffusivity $D_r \tau_r = D_r / (2\gamma) = 0.05$. The radial distribution $\tilde{\rho}_s(r)$ is computed by numerically solving the dimensionless version of the Langevin equations (1) (solid lines) and from eq. (8) (dashed lines). (b) Transition from weak to strong trapping at constant $Pe = 20$ by varying the rotational diffusivity D_r from 10 to 400. The dashed lines belong to eq. (12). Inset: critical $D_r^{(c)}$ marking the transition from strong to weak trapping *vs.* Pe at three different γ . Symbols: numerically determined critical $D_r^{(c)}$; solid lines: fit of the numerical data to $\sim C_1 + C_2 e^{-C_3 Pe}$.

is much larger than the run-up time $\tau_r = 1/(2\gamma) = 0.05$, the analytical density perfectly agrees with the numerical results. The transition from strong to weak trapping occurs at $Pe = 2\sqrt{10} \approx 6$. Figure 1(b) demonstrates the transition from weak to strong trapping as the rotational diffusivity D_r is gradually increased at fixed $Pe = 20$. Reasonable agreement between eq. (12) (dashed lines) and the numerical solution is expected for $D_r > Pe^2/2 = 200$.

The inset in fig. 1(b) shows the numerically computed critical $D_r^{(c)}(Pe)$, which marks the transition from strong to weak trapping at three different values of γ . Remarkably, $D_r^{(c)}(Pe)$ remains finite even when the Péclet number becomes very large. This can be explained as follows. The characteristic time, which is needed for the particle to reverse the direction of its active motion, is approximated by π^2/D_r . If this time is much smaller than the run-up time $\tau_r = 1/(2\gamma)$ in the potential $U = \gamma r^2$, we expect a bell-shaped radial distribution centered at $r = 0$. Consequently, the critical rotational diffusivity $D_r^{(c)}$ at large Pe is found to be proportional to γ , namely $D_r^{(c)} \sim \gamma$. This result is in agreement with the findings presented in the inset of fig. 1(b).

Dynamic density functional theory of interacting active particles. – As pointed out in the introduction, the main obstacle towards constructing a DDFT for active particles is the unknown effective excess free energy functional $F_{\text{ex}}[\rho(\mathbf{r}, \mathbf{p}, t)]$, which describes particle interactions or their correlations in terms of the one-body density $\rho(\mathbf{r}, \mathbf{p}, t)$. Rather than trying to pursue the highly complicated task of computing $F_{\text{ex}}[\rho(\mathbf{r}, \mathbf{p}, t)]$, we directly derive

an effective Smoluchowski equation for the one-particle distribution function averaged over the rotational degree of freedom. Thereby we demonstrate a systematic way of approximately describing the spatial dynamics of interacting active particles in 2D traps. To this end, we map the system of active particles onto a system of passive colloids moving in an effective trapping potential. The latter is computed using the analytical steady-state densities of non-interacting particles found in the previous section.

We consider N active particles in a radially symmetric 2D trapping potential $U(r)$. The particles interact via the two-body purely steric potential $w(|\mathbf{r}_i - \mathbf{r}_k|)$. For any pair of particles (i, k) , their directions of motion, \mathbf{p}_i and \mathbf{p}_k , remain unaffected by the interaction. For vanishing propulsion velocity $v_0 \rightarrow 0$, the system reduces to the case of passive particles, for which the equilibrium excess free energy F_{ex} as a function of the one-body density exists.

Following refs. [9,18], one can integrate the Smoluchowski equation for the N -body density over the coordinates and directions of motion of $(N-1)$ particles and ultimately obtain an equation for the one-particle density $\rho(\mathbf{r}, \mathbf{p}, t)$, normalized to $\int \rho d\mathbf{r} d\mathbf{p} = N$:

$$\partial_t \rho + \nabla \cdot \mathbf{J}_t^m + \mathbf{R} \cdot \mathbf{J}_{\text{rot}} = 0. \quad (13)$$

Here we have introduced the translational flux $\mathbf{J}_t^m = -[\mu \nabla \delta F_{\text{ex}}[\rho] / \delta \rho + v_0 \mathbf{p} - \mu \nabla U(r)] \rho - \mu k_B T \nabla \rho$ and the rotational flux $\mathbf{J}_{\text{rot}} = -D_r \mathbf{R} \rho$. The interaction between the particles is taken into account via the excess free energy $F_{\text{ex}}[\rho]$. Since the particle interactions do not depend on the velocity directions \mathbf{p} , we assume that $F_{\text{ex}}[\rho] = \int \Phi(\{\Pi(\mathbf{r})\}) d\mathbf{r}$, where $\Phi(\{\Pi(\mathbf{r})\})$ is the free energy density in terms of the positional distribution function $\Pi(\mathbf{r}) = \int \rho(\mathbf{r}, \mathbf{p}) d\mathbf{p}$.

We derive an equation for $\Pi(\mathbf{r})$ by integrating eq. (13) over all possible directions \mathbf{p} and by using $\int \mathbf{R} \cdot \mathbf{J}_{\text{rot}} d\mathbf{p} = 0$:

$$\partial_t \Pi + \nabla \cdot \int \mathbf{J}_t^m(\mathbf{r}, \mathbf{p}) d\mathbf{p} = 0. \quad (14)$$

Since $\delta F_{\text{ex}}[\rho] / \delta \rho = \delta F_{\text{ex}}[\Pi] / \delta \Pi$, one immediately obtains for the term containing the excess free energy, $\int \rho \nabla \delta F_{\text{ex}}[\rho] / \delta \rho d\mathbf{p} = \Pi \nabla \delta F_{\text{ex}}[\Pi] / \delta \Pi$.

The only remaining term in eq. (14) that depends on \mathbf{p} is the local average direction of motion $\langle \mathbf{p} \rangle = \int \mathbf{p} \rho d\mathbf{p}$. Taking into account that particle interactions do not influence the velocity direction \mathbf{p} , we approximate $\langle \mathbf{p} \rangle$ using the stationary distribution functions $\rho_s(\mathbf{r}, \psi)$ of the single-particle case given by eqs. (7) and (11) to compute the average. The azimuthal component of $\langle \mathbf{p} \rangle = \int \mathbf{p} \rho_s d\mathbf{p}$ vanishes exactly. In our dimensionless units, we obtain for the radial component of $\langle \mathbf{p} \rangle$ in case of small (s) and large (l) rotational diffusivities the respective averages

$$\langle \mathbf{p} \rangle_r^{(s)} = \tilde{\rho}_s^{(0)}(r) Pe \frac{I_1(Pe r)}{I_0(Pe r)}, \quad (15)$$

$$\langle \mathbf{p} \rangle_r^{(l)} = \tilde{\rho}_s(r) Pe \frac{Pe \partial_r U(r)}{2D_r + Pe^2 U(r)}. \quad (16)$$

On substituting the radial densities on the r.h.s of eqs. (15) and (16) by the non-stationary spatial distribution $\Pi(\mathbf{r}, t)$, we extend eqs. (15) and (16) towards the many-particle case,

$$\langle \mathbf{p} \rangle_r(t) = -\Pi(\mathbf{r}, t) \partial_r V(r)^{(s,l)}. \quad (17)$$

We have introduced radially symmetric potentials at small (s) and large (l) rotational diffusivities,

$$V(r)^{(s)} = -\ln I_0(\text{Pe } r), \quad (18)$$

$$V(r)^{(l)} = -\ln \left(1 + \frac{\text{Pe}^2 U(r)}{2D_r} \right). \quad (19)$$

Equation (17) implies that the system of active particles can be mapped onto a system of passive particles with the effective radially symmetric potential $W^{\text{eff}}(r)^{(s,l)} = U(r) + V(r)^{(s,l)}$. The dimensionless Smoluchowski equation (14) can now be written in the typical form of DDFT:

$$\partial_t \Pi = \nabla \cdot \left[\Pi \nabla \frac{\delta F[\Pi]}{\delta \Pi} \right], \quad (20)$$

where we have introduced the standard form of the DFT free energy functional $F[\Pi] = F_{\text{ex}}[\Pi] + \int \Pi (\ln \Pi - 1) d\mathbf{r} - \int W^{\text{eff}}(r)^{(s,l)} \Pi d\mathbf{r}$.

In order to test the accuracy of the developed effective DDFT for active particles, we consider active hard discs of the diameter d , interacting via standard hard-core repulsive potential $w_{\text{hc}}(|\mathbf{r}_i - \mathbf{r}_k|)$. For passive hard discs analytic expressions for the equilibrium excess free energy F_{ex} exist. They are given by the various forms of the Rosenfeld functional in terms of the packing fraction or one-body density [24–26]. We numerically integrate the Langevin equations of N active particles in a harmonic trap $U(r) = \gamma r^2$ interacting via the hard-core repulsive potential w_{hc} . The results are compared with Brownian dynamics simulations of a system of passive hard discs moving in the effective external potential $W^{\text{eff}}(r)$. We emphasize since the Rosenfeld excess free energy functional F_{ex} is pretty accurate, we expect the stationary solution of eq. (20) to coincide with the results from the Brownian dynamics simulations.

Figure 2 shows the stationary radial one-body density $\Pi_s(r)/N$ as obtained for $N = 50$ particles for different values of the Péclet number Pe given in the legend. The rest of the parameters are $D_r = 0.04$ and $\gamma = 2$, meaning limit of small diffusivity, $D_r/\gamma \ll 1$. Solid lines correspond to the radial distribution of active particles interacting via the hard-core potential w_{hc} in the harmonic trapping potential $U = \gamma r^2$. For comparison, dashed lines represent the distribution of passive hard discs moving in the effective potential $W^{\text{eff}}(r)^{(s)} = U(r) + V(r)^{(s)}$ with $V(r)^{(s)}$ from eq. (18).

In case of strong confinement ($\text{Pe} < \sqrt{4\gamma} \approx 2.8$), passive hard discs form a compact cluster in the center of the trap (see $\Pi_s(r)$ at $\text{Pe} = 1$ in fig. 2). Within the cluster, the particles are arranged in concentric circles giving rise to

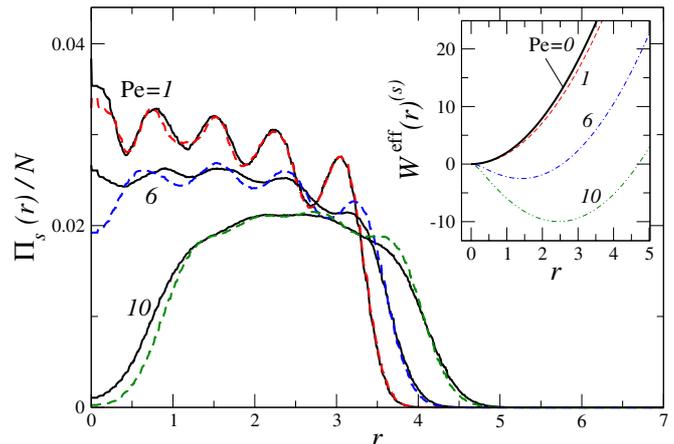


Fig. 2: (Color online) Stationary radial distribution function $\Pi_s(\mathbf{r})/N$ for different Péclet numbers Pe . They are obtained from solving the Langevin equations for $N = 50$ particles numerically: solid lines represent the system of active particles interacting via the hard-core potential w_{hc} in the harmonic trap $U = \gamma r^2$; dashed lines represent the passive hard discs in the effective potential $W^{\text{eff}}(r)^{(s)}$ with $V(r)^{(s)}$ from eq. (18). Other parameters are $D_r = 0.04$ and $\gamma = 2$. Inset: the effective potential $W^{\text{eff}}(r)^{(s)}$ at different Péclet numbers. Note that at $\text{Pe} = 0$, $W^{\text{eff}}(r)^{(s)} = U(r)$ (thick solid line).

undulations of the density with the typical period which is given by the minimal distance between particles. In order to overcome technical difficulties in dealing with the pure hard-core repulsive potential w_{hc} , we have used in our simulations an effective soft-core potential of the form $w = (1/30)(d/|\mathbf{r}_i - \mathbf{r}_k|)^{30}$ [28,29]. As a consequence, the minimal distance between particles, which we interpret as an effective diameter d_{eff} , was γ -dependent and generally less than d [30]; for instance, $d_{\text{eff}} \approx 0.75$ at $\gamma = 2$. This gives rise to a typical packing fraction which we estimated as $\sim (50d_{\text{eff}}^2)/(4R^2) \approx 0.4, \dots, 0.5$, where R was the characteristic radius of the cluster.

The effect of the active motion on the radial distribution is visualized in fig. 2 by gradually increasing the Péclet number Pe . The activity of the particles within the cluster, increases with Pe leading to a broader cluster. Remarkably, the effective DDFT given by the dashed lines in fig. 2 reproduces extremely well the exact distribution at small $\text{Pe} = 1$ corresponding to a very high packing fraction and strong confinement. At $\text{Pe} = 10$ or weak confinement the agreement is also very good with deviations at the center and the edge of the distribution. Even at intermediate values of Pe the overall shape of the distribution function is reproduced by the effective DDFT, whereas it fails to reproduce details in the oscillations.

We explain our findings as follows. At small Pe we expect that the active motion of the particles does not significantly influence the local ordering of the particles which is enforced by the trapping potential $U(r)$ to which the active motion-induced potential $V(r)^{(s)}$ contributes a disturbance. Indeed, the inset of fig. 2 shows that

$W^{\text{eff}}(r)^{(s)}$ at $\text{Pe} = 1$ almost coincides with $U(r)$. On the other hand, for large Pe or at weak confinement the cluster expands and the local packing fraction decreases. So we expect our approximation of determining the average direction of motion $\langle \mathbf{p} \rangle$ from the single-particle case to be valid. At intermediate Péclet numbers such as $\text{Pe} = 6$ the potential $W^{\text{eff}}(r)^{(s)}$ differs significantly from $U(r)$. The packing fraction is still sufficiently large so that the single-particle approximation for $\langle \mathbf{p} \rangle$ only determines the overall shape of the distribution. However, it fails to reproduce the local details which depend on the particle correlations.

We close with a final comment. In the limit of vanishing Péclet number or activity of the particles, $V(r)^{(s)}$ in eq. (18) vanishes and the effective potential $W^{\text{eff}}(r)^{(s)}$ approaches the original trapping potential $U(r)$. So, we are dealing with a system of passive particles. However, also for sufficiently large rotational diffusivity D_r , the potential $V(r)^{(l)}$ in eq. (19) vanishes and again we recover the case of purely passive particles. Here, the rotational diffusion is so large that the active motion does not influence the behavior of the particle suspension.

Conclusion. – We have studied the dynamics of active particles in a 2D trap which we mimic by a radially symmetric trapping potential. We have used this model system to formulate an effective theory for the one-particle spatial density where the interacting active particles are mapped on a system of passive circular particles that move in an effective trapping potential. To arrive at such a formulation, we first derived analytic expressions for the stationary distribution of a single active particle in the limit of small and large rotational diffusivity. We then addressed interacting active particles starting from the integrated Smoluchowski equation for the one-particle density. Particle interactions were taken into account by the excess free energy as it is usually done in any DDFT. Assuming that the orientations of the circular active particles are mainly governed by the trapping potential, we calculated their mean orientation using the stationary distribution of a single active particle. This enabled us to introduce an effective external potential which encodes the active motion of the particles. Finally, we formulated the dynamics of the one-particle spatial distribution in form of a conventional DDFT for passive particles moving in the effective trapping potential. The accuracy of the developed approach was tested on the example of active hard discs trapped in a harmonic potential. Brownian dynamics simulations for both the original system of active discs interacting by a soft-core potential and passive discs in the effective trapping potential show a remarkable agreement in the stationary one-particle distribution. Only at intermediate Péclet numbers differences are visible on the length scale of the particle diameter.

Our work clearly identifies different contributions to the collective motion of spherical microswimmers and thereby suggests an effective dynamic theory for the one-particle

distribution. Future work will address active particles with an elongated shape and include hydrodynamic interactions.

AP thanks the Research Training Group 1558 funded by Deutsche Forschungsgemeinschaft for financial support.

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